Tableau 2. *Principales distances interatomiques* (Å), *angles des liaisons* (°) *et écarts-type*

Ca–O(1)	2,308 (1)	O(4)–C(4)	1,234 (2)
Ca–O(2^{i})	2,334 (2)	N–C(3)	1,454 (2)
Ca–O(4^{ii})	2,306 (1)	N–C(4)	1,330 (2)
S–O(1)	1,444 (1)	C(1)–C(2)	1,512 (3)
S–O(2)	1,451 (2)	C(2)–C(3)	1,520 (3)
S–O(3)	1,438 (2)	C(4)–C(5)	1,492 (3)
S–C(1)	1,769 (2)		
O(1)–Ca–O(2^{i})	89,38 (5)	O(3)–S–C(1)	106,7 (1)
O(1)–Ca–O(4^{ii})	92,11 (5)	C(3)–N–C(4)	123,6 (2)
O(2^{i})–Ca–O(4^{ii})	88,68 (6)	S–C(1)–C(2)	111,9 (1)
O(1)–S–O(2)	112,35 (9)	C(1)–C(2)–C(3)	113,2 (2)
O(1)–S–O(3)	112,43 (9)	N–C(3)–C(2)	112,8 (2)
O(1)–S–C(1)	106,7 (1)	O(4)–C(4)–N	121,4 (2)
O(2)–S–O(3)	112,7 (1)	O(4)–C(4)–C(5)	121,9 (2)
O(2)–S–C(1)	105,40 (9)	N–C(4)–C(5)	116,7 (2)

Code de symétrie: (i) $1+x, y, z$; (ii) $1+x, y, 1+z$.

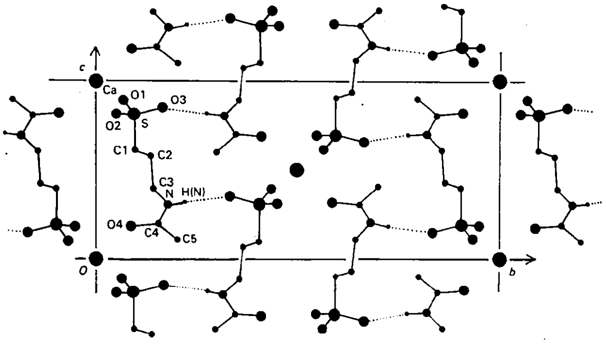

Fig. 1. Dessin de la structure vue selon [100] et noms des atomes. Les traits en pointillé représentent les liaisons hydrogène.

(hydroxy-2 éthyl)taurine (Galešić, Herceg & Matković, 1981). Etude cristallographique et vibrationnelle de la glycyltaurine (Garrigou-Lagrange, Jensen & Cotrait, 1977). Etude clinique du bis(acétamido-3 propanesulfonate-1) de calcium (Lhuintre, Moore, Saligaut, Boismare, Daoust, Chrétien, Tran & Hillemand, 1985).

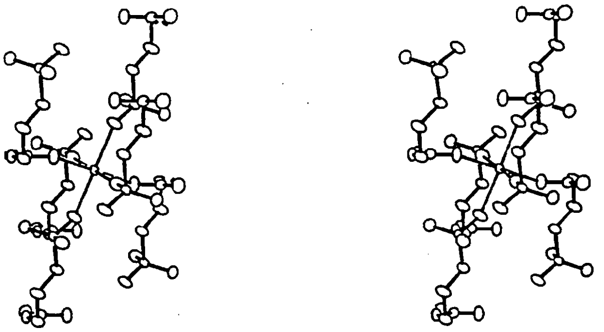

Fig. 2. Vue stéréoscopique de l'environnement de l'ion Ca^{2+}.

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Structure of 1,4-Difluoro-1,1,4,4-tetranitro-2,3-butanediyl Diacetate

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(*Received* 17 *December* 1987; *accepted* 15 *March* 1988)

Abstract. $C_8H_8F_2N_4O_{12}$, $M_r = 390{\cdot}17$, monoclinic, $P2_1/n$, $a = 6{\cdot}069\ (1)$, $b = 12{\cdot}117\ (2)$, $c = 10{\cdot}175\ (1)$ Å, $\beta = 93{\cdot}98\ (1)°$, $V = 746{\cdot}5\ (2)$ Å^3, $Z = 2$, $D_x = 1{\cdot}736$ Mg m^{-3}, $\lambda(\mathrm{Cu}\ K\alpha) = 1{\cdot}54178$ Å, $\mu = 1{\cdot}57$ mm^{-1}, $F(000) = 396$, $T = 295$ K, final $R = 0{\cdot}035$, $wR = 0{\cdot}053$ for 1120 observed reflections. The molecule lies on a center of symmetry. Crowding in the vicinity of the nitro groups is evidenced by the eclipsed

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Table 1. *Atomic coordinates* (× 10^4) *and equivalent isotropic displacement parameters* ($Å^2 \times 10^3$)

	x	y	z	U_{eq}*
F	1291 (2)	4696 (1)	3876 (1)	48 (1)
N(1)	3764 (3)	3485 (1)	3025 (2)	44 (1)
O(1*a*)	2876 (3)	3774 (2)	1987 (1)	69 (1)
O(1*b*)	5311 (3)	2873 (1)	3209 (2)	65 (1)
N(2)	1631 (3)	3001 (1)	4902 (2)	46 (1)
O(2*a*)	2819 (3)	2279 (1)	5365 (2)	68 (1)
O(2*b*)	−347 (3)	3053 (1)	4890 (2)	71 (1)
C(1)	2820 (3)	3966 (1)	4267 (2)	36 (1)
C(2)	4571 (3)	4449 (1)	5252 (2)	33 (1)
O(2)	3463 (2)	4670 (1)	6409 (1)	36 (1)
O(3)	5698 (3)	3510 (1)	7607 (2)	67 (1)
C(3)	4165 (4)	4125 (2)	7566 (2)	44 (1)
C(4)	2759 (6)	4458 (2)	8632 (2)	60 (1)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

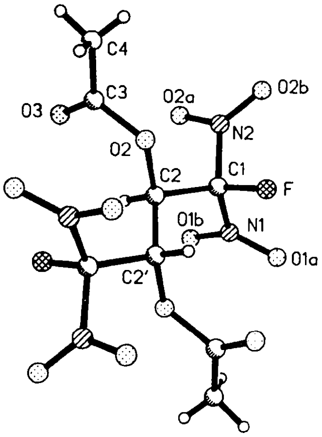

Fig. 1. Perspective drawing of the results of the X-ray study on the substituted butane.

Table 2. *Bond lengths* (Å) *and bond angles* (°)

F—C(1)	1·323 (2)	N(1)—O(1*a*)	1·204 (2)
N(1)—O(1*b*)	1·201 (2)	N(1)—C(1)	1·538 (2)
N(2)—O(2*a*)	1·208 (2)	N(2)—O(2*b*)	1·202 (2)
N(2)—C(1)	1·541 (2)	C(1)—C(2)	1·526 (2)
C(2)—O(2)	1·421 (2)	O(2)—C(3)	1·392 (2)
O(3)—C(3)	1·190 (2)	C(3)—C(4)	1·481 (3)
C(2)—C(2′)	1·535 (2)		
O(1*b*)—N(1)—O(1*a*)	127·9 (2)	C(1)—N(1)—O(1*a*)	116·1 (2)
C(1)—N(1)—O(1*b*)	116·0 (2)	O(2*b*)—N(2)—O(2*a*)	127·7 (2)
C(1)—N(2)—O(2*a*)	115·4 (2)	C(1)—N(2)—O(2*b*)	116·9 (2)
N(1)—C(1)—F	107·5 (1)	N(2)—C(1)—F	107·1 (1)
N(2)—C(1)—N(1)	105·6 (1)	C(2)—C(1)—F	112·6 (1)
C(2)—C(1)—N(1)	113·8 (1)	C(2)—C(1)—N(2)	109·9 (1)
O(2)—C(2)—C(1)	105·6 (1)	C(3)—O(2)—C(2)	118·5 (1)
O(3)—C(3)—O(2)	121·2 (2)	C(4)—C(3)—O(2)	109·4 (2)
C(4)—C(3)—O(3)	129·3 (2)	C(1)—C(2)—C(2′)	110·5 (2)
C(1)—C(2)—O(2)	105·6 (1)	O(2)—C(2)—C(2′)	107·7 (2)

geometry and close intramolecular approaches of the F and O atoms [F···O(1*a*) 2·47 and F···O(2*b*) 2·48Å]. There are also close N···O intramolecular approaches [N(2)···O(2) 2·73 and N(1)···O(2′) 2·83 Å].

Experimental. Colorless, 0·17 × 0·23 × 0·50 mm crystal synthesized and crystallized by William Koppes of the Naval Surface Weapons Center, Silver Spring, Maryland, USA. Automated Nicolet *R*3*m* diffractometer with incident-beam graphite monochromator; 25 centered reflections within $50 \leq 2\theta \leq 66°$ used for determining cell parameters. Data corrected for Lorentz and polarization effects, but not for absorption. $2\theta_{max} = 125°$; range of *hkl*: $0 \leq h \leq 6$, $0 \leq k \leq 13$, $-11 \leq l \leq 11$; standards, 420, 006, 06$\bar{2}$, monitored every 100 reflections with random variation of 2·3% over data collection; $\theta/2\theta$ mode, scan width $[2\theta(K\alpha_1) - 1{\cdot}0]$ to $[2\theta(K\alpha_2) + 1{\cdot}0]°$, scan rate a function of count rate (8° min^{-1} minimum, 30° min^{-1} maximum; 1460 reflections measured, 1189 unique, $R_{int} = 0{\cdot}011$, 1120 observed $[F_o > 3\sigma(F_o)]$.

Structure solved by direct methods. The least-squares refinement used the full-matrix program provided with the MicroVax version of the *SHELXTL* system (Sheldrick, 1980). $\sum w(|F_o| - |F_c|)^2$ minimized where $w = 1/[\sigma^2(|F_o|) + g(F_o)^2]$, $g = 0{\cdot}00024$, secondary isotropic extinction from $F_c^* = F_c/[1{\cdot}0 + 0{\cdot}002(p)F_o^2/\sin 2\theta]^{0{\cdot}25}$ where $p = 0{\cdot}014$ (3). 135 parameters were refined: atom coordinates for all atoms, anisotropic temperature factors for non-H atoms and isotropic temperature factors for H atoms; $(\Delta/\sigma)_{max} = 0{\cdot}01$, $R = 0{\cdot}035$, $wR = 0{\cdot}053$, $S = 2{\cdot}44$. Final difference Fourier map excursions 0·18 and −0·17 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).† Atom numbering for Tables 1 and 2 (atom coordinates, bond distances and bond angles) follows that shown in Fig. 1.

Related literature. The structures of other compounds containing nitro groups and F atoms have been reported (Koppes, Chaykovsky, Adolph, Gilardi & George, 1987).

This work was supported in part by contract No. N00173-86-M-R828 from the ONR Mechanics Division.

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† Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44904 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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